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Pedro F. Embid

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Department of Mathematics
The University of New Mexico
Albuquerque, NM 87131

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This work provides a mathematical analysis of a reactive mutiphase flow model introduced by Baer and Nunziato in their studies of deflagration-to detonation transition (DDT) in reactive granular materials. This work combines asymptotic methods with numerical computations and theoretical analysis. In particular, we derive an asymptotic model to explain the formation and growth of hot spots during DDT in reactive granular materials. The model is founded on nonlinear geometrical optics and high energy asymptotics near choked flow states. Through analysis and numerical simulations, the model is able to reproduce several of the scenarios for DDT previously documented in the literature for the continuum model of Baer and Nunziato.

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Final Report

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Principal Investigator: Pedro F. Embid

Address: Department of Mathematics and Statistics
The University of New Mexico
Albuquerque, NM 87131

Phone: (505)277-2114

Fax: (505)277-5505

e-mail: pembid@snell.unm.edu.

Abstract

This work provides a mathematical analysis of a reactive multiphase flow model introduced by Baer and Nunziato in their studies of deflagration-to-detonation transition (DDT) in reactive granular materials. This work combines asymptotic methods with numerical computations and theoretical analysis. In particular, we derive an asymptotic model to explain the formation and growth of hot spots during DDT in reactive granular materials. The model is founded on nonlinear geometrical optics and high energy asymptotics near choked flow states. Through analysis and numerical simulations, the model is able to reproduce several of the scenarios for DDT previously documented in the literature for the continuum model of Baer and Nunziato.

Introduction

Understanding the phenomena involved in the deflagration-to-detonation transition (DDT) of reactive granular materials has fundamental relevance for the industry and the military. For example, issues related to DDT are present when manufacturing and handling high explosives, gun propellants and solid roket propellants.

Baer and Nunziato [2] introduced a system of seven partial differential equations to study DDT in reactive two-phase flows. The model is based on the continuum theory of mixtures and the second law of thermodynamics. This continuum model gave good quantitative agreement with experimental measurments of important parameters such as flame speed and run-to-detonation lenghts for the explosives HMX and CP [1, 2]. In addition, the numerical experiments on the Baer-Nunziato model document various possible scenarios for DDT depending on the imposed initial and boundary conditions [1, 2, 3]. These scenarios include: 1. Formation and growth of hot spots behind and moving away from the the compaction front. 2. Formation and growth of hot spots within the compaction front. 3. Failure to produce hot spots and no transit to detonation.

The objective of the research funded by this grant was to study mathematically the continuum model in order to provide insight into the physics of multiphase flow and the DDT phenomena. Specifically, we concentrated our efforts in the following topics: 1. Transition to detonation in reactive multiphase flows. 2. Structure of detonation waves for reactive multiphase flows. The results of the research funded by this grant are described below.

Transition to detonation in reactive multiphase flows

The continuum system of reactive multiphase flow is very complex because of the many state variables it describes: density, pressure, velocity and volume fraction for both phases, and the many transport mechanisms involved for the phase interactions: chemical reaction, heat convection, drag, and diffusion. To study mathematically the DDT process directly in the continuum system would be very difficult. Instead, the objective of this work was to derive in a rational fashion a simplified asymptotic model that captures the relevant physical mechanisms and is able to explain the formation and growth of hot spots documented in the numerical experiments [1, 2, 3].

The characteristics analysis we did for the system [4, 5] revealed the existence of special singular points for the flow. These singular points correspond physically to *choked flow* states where the speed of the gas relative to the solid becomes sonic, i.e. $v_s = v_g \pm c_g$. Mathematically, near regions of choked flow there is substantial resonant interaction between one of the gas-acoustic modes and the compaction mode which is moving at the speed of the solid. In [5] we exploited this resonant behavior to derive a simplified asymptotic system of equations capable of describing the formation and growth of hot spots in reactive

multiphase flows. This asymptotic system is valid near choked flow states and near ignition temperature conditions for the solid explosive. It also incorporates the effects of compaction and gas-acoustic resonances together with heat convection effects between the solid and the hot product gases, and the chemical reaction of the solid grains.

The derivation of the model is based on the method of nonlinear geometrical optics near a uniform choked flow background state, and combined with high energy asymptotics near the ignition temperature condition for the solid. In addition, the derivation of the asymptotic model in [5] is presented in a general abstract setting so that it should be useful in other potential applications in multiphase flow technology.

The resulting asymptotic model derived in [5] is

$$\begin{aligned} \frac{\partial \sigma_1}{\partial t} + \frac{\partial}{\partial \theta}\left((a+bt)\sigma_1 + c_1\frac{\sigma_1^2}{2}\right) &= \frac{\partial \sigma_2}{\partial \theta} \ , \\ \frac{\partial \sigma_2}{\partial t} + c_2\frac{\partial \sigma_2}{\partial \theta} &= R\exp(\alpha_1\sigma_1 + \beta_1 + \beta_2 t) \ . \end{aligned}$$

Here σ_1 is the gas-acoustic perturbation amplitude, and σ_2 is the compaction amplitude. t is time and θ measures the distance from the compaction front, scaled through the asymptotics. The remaining parameters a, b, c_1, c_2, α_1, β_1, and β_2 are constants evaluated at the background state; they incorporate important effects of heat convection transfer between the gas and solid phases, and the burning of the grains.

In [6] we employed the above asymptotic model to predict in qualitative fashion the scenarios documented numerically in [1, 2, 3] for the birth and growth of hot spots in reactive granular flows. In our analysis we studied the interaction of a small amplitude burning compaction wave with an initially uniform gas state. The different regimes described in [1, 2, 3] can be obtained with suitable restrictions on the signs and magnitudes of the parameters b and β_2; these restrictions are easy to verify and are naturally related to the background state. In particular, these restrictions describe whether the gas is preheating the solid explosive and thus enhancing combustion, and whether the temperatures of the gas and the solid are very disparate. More precisely, in [4] we showed the following: 1. For $\beta_2 > 0$, $b < 0$, and b moderately large in magnitude, a growing hot spot develops behind the compaction front, and it moves away from the compaction front. 2. For $\beta_2 > 0$, $b < 0$, and b small in magnitude, a hot spot develops and grows within the compaction front; and 3. for $\beta_2 < 0$ no hot spot develops and the result is essentially identical to a nonreactive

moving wave. All these results are in qualitative agreement with the numerical scenarios for DDT documented in [1, 2, 3]. This last spring the author was invited by J. Bdzil to deliver a lecture on DDT at Los Alamos National Laboratories. We presented at that time the results described above and they were received with great interest by the present audience.

Currently I am working on performing direct numerical comparisons between the asymptotic model and the Baer-Nunziato model in order to obtain a quantitative validation of the asymptotic theory.

Structure of detonation waves for reactive multiphase flows

The study of the structure of detonation waves is fundamental to understand the terminal stage of DDT when the detonation wave is fully developed. One of our objectives is to study the structure of the detonation wave in the absence of diffusive effects, i.e. the extension of the ZND theory to multiphase reactive flows. Then we add the effects of diffusive transport and consider diffusive detonation waves.

In the ZND theory the chemical reaction is triggered by the passing of a non-reactive shock wave. Therefore a basic ingredient in this theory is to determine the possible states connected by non-reactive shocks in the multiphase flow system. In [4] we characterized most of those states. However, it still remains to characterize all the possible non-reactive shocks that propagate at speed v_s. This issue is important for the study of burning fronts propagating at the solid speed. In addition, the equations governing the structure of detonation waves for reactive multiphase flow involve seven nonlinear, coupled ordinary differential equations whose analytic treatment is difficult. For this reason we are currently studying the structure of detonation waves for the asymptotic model instead of the continuum model. For the symptotic model we only need to study a set of two nonlinear and non-autonomous ordinary differential equations for which we are applying phase plane techniques. This analysis should provide a simpler but qualitatively equivalent picture of the structured detonation waves. This information can then be used as guidance for the continuum model.

Conclusions

The research funded by this grant provided the following results: 1. Development of simplified asymptotic models for DDT reactive multiphase flows, and with possible applications

to other areas in multiphase flow technology [5]. 2. A theory for hot spot formation and transition to detonation in reactive granular flows [6]. 3. The analysis in [4] provides a variety of elementary exact solutions of the continuum system that are useful as test problems for the existing numerical solution methods, as well as being neccesary building blocks in the solution of the Riemann problem, and the design of Godunov-type numerical schemes for the multiphase flow equations. Finally, we will continue research in the direct quantitative comparison of the asymptotic and the continuum model, and continue research on the problem of the structure of fully developed detonation waves.

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